shape_statistic

December 1, 2021

Implement metrics to compare two arbitrary distributions and apply to velocity profiles. Check the implementations for similarity by eye At the end we can add the velocity distribution similarity metric to our analysis (e.g. sobolnote.py)

[15]:
```
import sys, os
join = lambda *x: os.path.abspath(os.path.join(*x))
import numpy as np
import matplotlib.pyplot as plt
import matplotlib as mpl
import pili
import rtw
import _fj
import plotutils
import collections
import scipy.stats
import twanalyse
import pandas as pd
import parameters
import seaborn as sns
```

[16]:
```
# paths
notedir, notename = os.path.split(os.getcwd())
notedir, notename
root = pili.root
# candidate to compare against
print("loading experiment data")
all_idx, all_trs = _fj.slicehelper.load_linearized_trs("all")
flipped, scores = _fj.redefine_poles(all_trs)
reference_idx = _fj.load_subset_idx()
reftrs = {}
for key, subidx in reference_idx.items():
    reftrs[key] = [all_trs[idx] for idx in subidx]

print("finished")
```

```
 10%|          | 298/3113 [00:00<00:00, 2972.37it/s]
```

```
loading experiment data
```

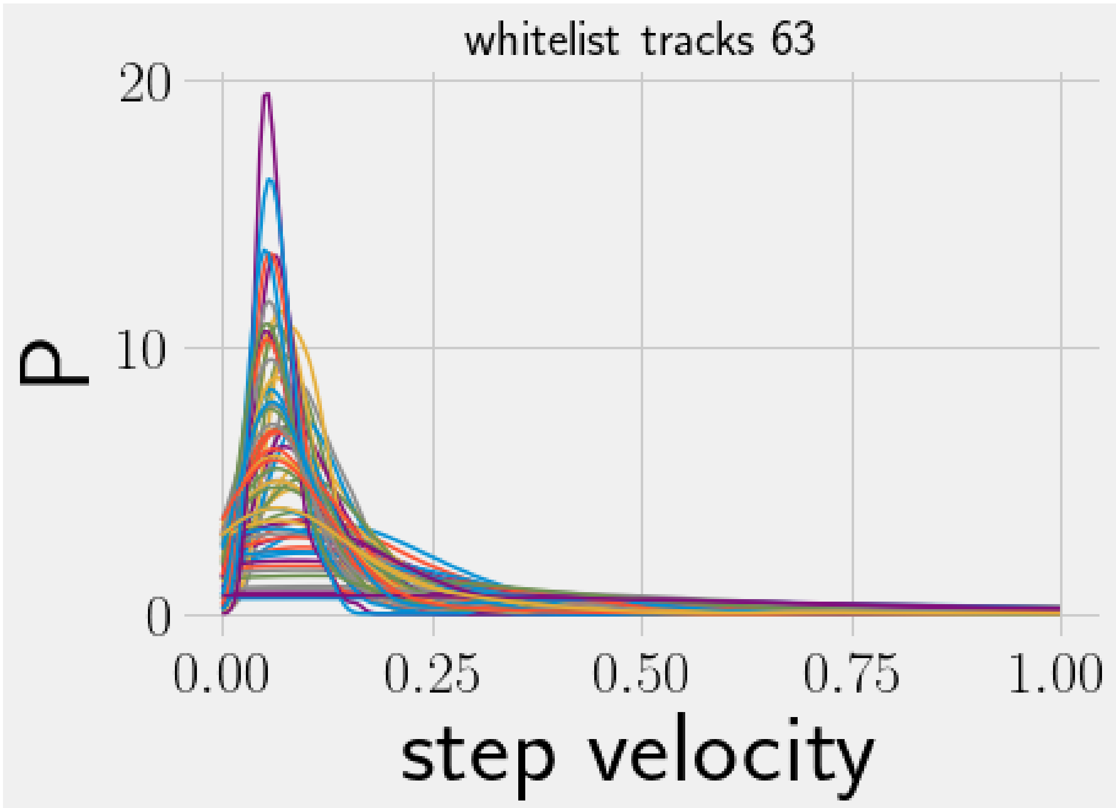
```
100%|          | 3113/3113 [00:01<00:00, 2142.74it/s]
/home/dan/.local/lib/python3.8/site-packages/numpy/core/fromnumeric.py:3419:
RuntimeWarning: Mean of empty slice.
  return _methods._mean(a, axis=axis, dtype=dtype,
/home/dan/.local/lib/python3.8/site-packages/numpy/core/_methods.py:188:
RuntimeWarning: invalid value encountered in double_scalars
  ret = ret.dtype.type(ret / rcount)
```

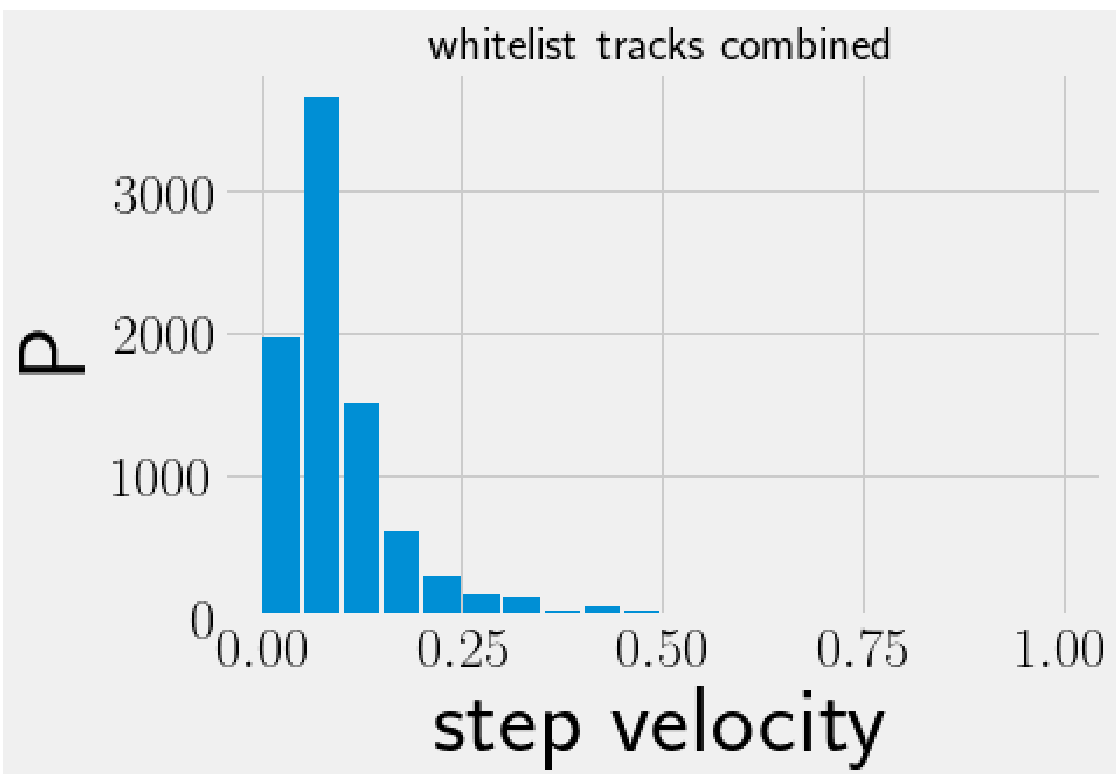
```
flipped 631/3113 tracks (20.3%)
finished
```

[17]:
```python
# simulation
angle1d_dir = join(root, "../run/new/angle_smoothed/range_pbrf")
simdata = collections.OrderedDict()
simdata[angle1d_dir] = rtw.DataCube(target=angle1d_dir)
```

[18]:
```python
# config
histstyle = {'rwidth': 0.9}
```

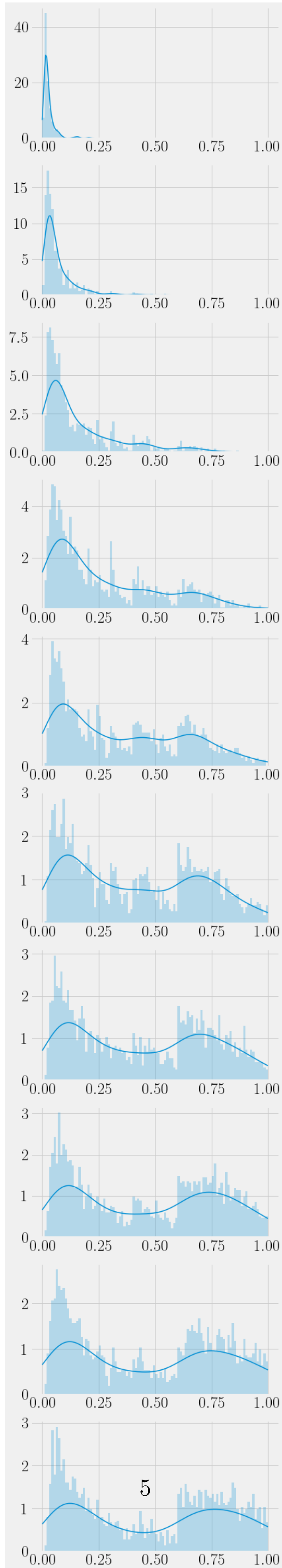
[19]:
```python
# plot individual track and combined distributions
fig,ax = plt.subplots(figsize=(6,4))
vellst = []
xlim = (0,1.0)
ax.set_title("whitelist tracks {}".format(len(reftrs["top"])))
for tr in reftrs["top"]:
    _vel = tr.get_step_speed()
    vellst.append(_vel)
    plotutils.ax_kdeplot(ax, _vel, xlims=xlim)
    ax.set_xlabel("step velocity")
    ax.set_ylabel("P")

fig,ax = plt.subplots(figsize=(6,4))
ax.set_title("whitelist tracks combined")
ref_vel = np.concatenate(vellst)
ax.hist(ref_vel, bins=20, range=xlim, **histstyle)
ax.set_xlabel("step velocity")
ax.set_ylabel("P")

plt.show()
```


whitelist tracks 63
P
step velocity
0
10
20
0.00
0.25
0.50
0.75
1.00

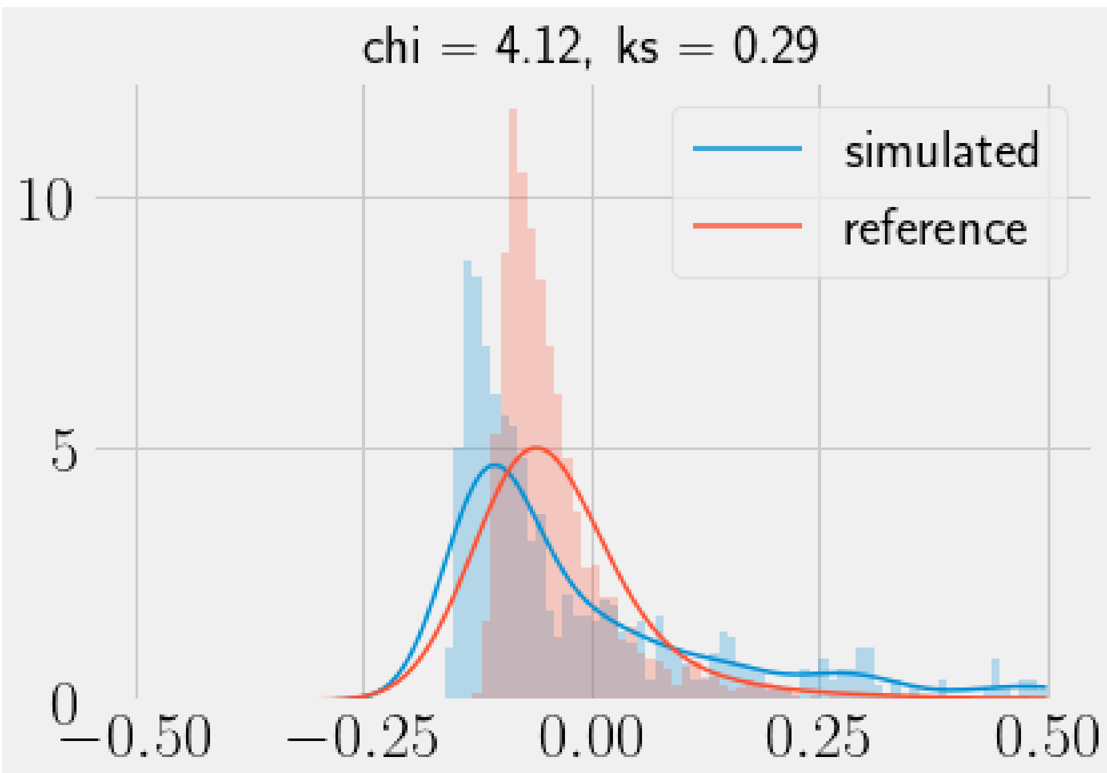

whitelist tracks combined
P
step velocity
0
1000
2000
3000
0.00
0.25
0.50
0.75
1.00

[20]:
```python
# plot velocity distributions for this 1d search
import readtrack
dc = list(simdata.values())[0]
print(str(dc))
trdata = dc.autocalculate(readtrack.trackset)
trdata = [[_fj.linearize(tr) for tr in trs] for trs in trdata]
vel = [np.concatenate([tr.get_step_speed() for tr in trs]) for trs in trdata]
nsteps = [np.sum([len(tr.step_idx) for tr in trs]) for trs in trdata]
print("nsteps", nsteps)
basis = dc.basis[0]

n = len(basis)
fig, axes = plt.subplots(n, figsize=(6,n*4))
# for i, value in list(enumerate(basis))[3:]:
for i, ax in enumerate(axes):
    plotutils.ax_kdeplot(ax, vel[i], xlims=xlim ,hist=True)
```

```
DataCube inspected directories at -->
/home/dan/usb_twitching/run/new/angle_smoothed/range_pbrf
parameters: ['anchor_angle_smoothing_fraction']
with shape: [10]
with basis:
anchor_angle_smoothing_fraction = [0.031, 0.062, 0.125, 0.25, 0.375, 0.5, 0.625,
0.75, 0.875, 1.0]
<--
nsteps [284, 519, 962, 1467, 1958, 2342, 2537, 2658, 2671, 2702]
```

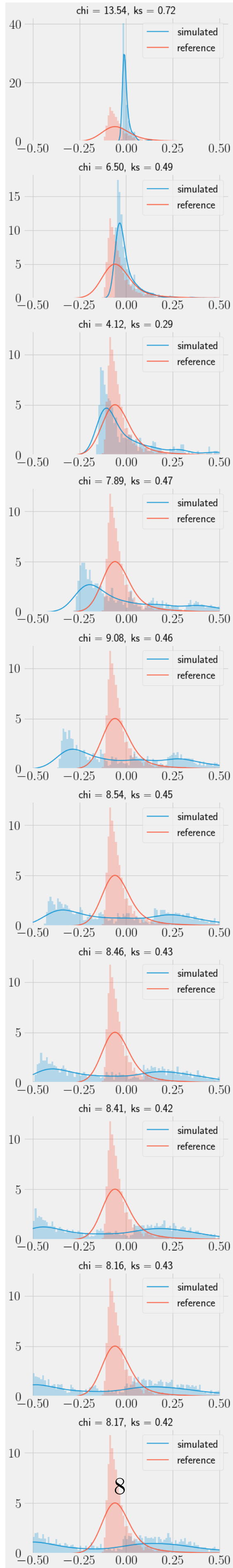

0 20 40
0.00 0.25 0.50 0.75 1.00
0 5 10 15
0.00 0.25 0.50 0.75 1.00
0.0 2.5 5.0 7.5
0.00 0.25 0.50 0.75 1.00
0 2 4
0.00 0.25 0.50 0.75 1.00
0 2 4
0.00 0.25 0.50 0.75 1.00
0 1 2 3
0.00 0.25 0.50 0.75 1.00
0 1 2 3
0.00 0.25 0.50 0.75 1.00
0 1 2 3
0.00 0.25 0.50 0.75 1.00
0 1 2
0.00 0.25 0.50 0.75 1.00
0 1 2 3
0.00 0.25 0.50 0.75 1.00

[21]:
```python
# superimise one simulated trajectory with the reference data
# def mean(x): return scipy.stats.trim_mean(x, 0.025)
mean = np.mean

def plot_similarity(ax, sim_vel, ref_vel):
    v1 = sim_vel - mean(sim_vel)
    v2 = ref_vel - mean(ref_vel)
    show_hist = True
    plotutils.ax_kdeplot(ax, v1, xlims=(-0.5,0.5), hist=show_hist)
    plotutils.ax_kdeplot(ax, v2, xlims=(-0.5,0.5), hist=show_hist)
    ax.legend(["simulated", "reference"])
    ks_statistic, pvalue = scipy.stats.ks_2samp(v1, v2)
    chi = twanalyse.chisquare(v1, v2)
    ax.set_title("chi = {:.2f}, ks = {:.2f}".format(chi, ks_statistic))

# test
i = 2
fig, ax = plt.subplots(figsize=(6,4))
plot_similarity(ax, vel[i], ref_vel)
```



[22]:

```python
# superimpose simulated data on reference data for the whole 1d range

n = len(basis)
fig, axes = plt.subplots(n, figsize=(6,n*4))
# for i, value in list(enumerate(basis))[3:]:
for i, ax in enumerate(axes):
    plot_similarity(ax, vel[i], ref_vel)
plt.tight_layout()
```


chi = 13.54, ks = 0.72
chi = 6.50, ks = 0.49
chi = 4.12, ks = 0.29
chi = 7.89, ks = 0.47
chi = 9.08, ks = 0.46
chi = 8.54, ks = 0.45
chi = 8.46, ks = 0.43
chi = 8.41, ks = 0.42
chi = 8.16, ks = 0.43
chi = 8.17, ks = 0.42
simulated
reference

If we need a reference for what these similarity numbers actually mean we can check back on this notebook We should be ready to add these metrics to our summary statistics

[23]:
```
# switch over to searching sobol dataset for the closest examples
import sobol
import twutils
simdir = "/home/dan/usb_twitching/run/b2392cf/cluster/sobol_01"
lookup = sobol.read_lookup(simdir)
problem = sobol.read_problem(simdir)
twutils.print_dict(problem)
_ , lduid = sobol.collect([], targetdir=simdir, alldata=True)
```


```
{
        "num_vars": 6,
        "names": [
                "k_ext_off",
                "dwell_time",
                "pilivar",
                "anchor_angle_smoothing_fraction",
                "k_spawn",
                "k_resample"
        ],
        "bounds": [
                [
                        0.2,
                        1.0
                ],
                [
                        0.5,
                        3.0
                ],
                [
                        1.0,
                        20.0
                ],
                [
                        0.125,
                        1.0
                ],
                [
                        0.5,
                        5.0
                ],
                [
                        1.0,
```

```
                        10.0
                    ]
            ]
}
```

[24]:

```
# load exp data
def _load_subset_speed():
    distrib = {}
    for name, ltrs in _fj.load_subsets().items():
        distrib[name] = np.concatenate([ltr.get_step_speed() for ltr in ltrs])
    return distrib
ref_vel = _load_subset_speed()
```

```
100%|      | 1/1 [00:00<00:00, 2898.62it/s]
100%|      | 63/63 [00:00<00:00, 6450.57it/s]
100%|      | 81/81 [00:00<00:00, 3940.09it/s]
100%|      | 79/79 [00:00<00:00, 1849.41it/s]
100%|      | 175/175 [00:00<00:00, 5294.04it/s]
```

[25]:

```
subsets = reference_idx.keys()
# scores = ['fanjin.%s.chi' % subset for subset in reference_idx.keys()]
scores = ['fanjin.%s.ks_statistic' % subset for subset in reference_idx.keys()]
Yf = sobol.collect_obs(lookup, lduid, subsets, scores)
def sortscore(problem, lookup, Yf, scores):
    # need to sort each column seperately, can't do this in one dataframe
    # construct a dataframe with cols [i, simulation_index, score] for each␣
↪subset
    paramlist = problem["names"]
    sortdf = {}
    for subset, data in Yf.items():
        sortidx = np.argsort(data)
        udir = [lookup[0][idx] for idx in sortidx]
        _cols = {"index": sortidx, "dir": udir, "score": data[sortidx]}
        _parlist = zip(problem["names"],  zip(*[lookup[1][_u] for _u in udir]))
        _cols.update({k:v for k, v in _parlist})
        _df = pd.DataFrame(_cols)
        sortdf[subset] = _df
    return sortdf
sortdf = sortscore(problem, lookup, Yf, scores)
sortdf["top"]
```

[25]:

	index	dir	score	k_ext_off	dwell_time	pilivar	\
0	5599	_u_4BvpMFSM	0.119646	0.451563	1.012695	1.185547	
1	5490	_u_bjwAuQOL	0.125704	0.357813	1.950195	2.669922	
2	5618	_u_cEN2qG75	0.126801	0.682813	2.555664	3.263672	
3	9935	_u_mcOorhHg	0.127497	0.232031	1.767090	6.733398	
4	9164	_u_7yd0LsJx	0.131379	0.250781	1.488770	13.747070	

```
…       …           …         …          …           …         …
14331      5  _u_SyQdaakH  0.819537  0.200000   0.500000   1.000000
14332    751  _u_GM4vF92B  0.820310  0.712500   0.695312  18.515625
14333  11728  _u_1179ubjo  0.822192  0.633594   2.738770  19.350586
14334      7  _u_L9q4zFIY  0.840073  0.200000   0.500000   1.000000
14335      2  _u_Af991wPr  0.852711  0.200000   0.500000   1.000000

       anchor_angle_smoothing_fraction   k_spawn  k_resample
0                             0.157471  4.323242    5.025391
1                             0.160889  3.602539    9.103516
2                             0.184814  4.586914    8.259766
3                             0.142944  4.248535    7.565430
4                             0.163452  4.283691    8.338867
…                                  …         …           …
14331                         0.125000  0.500000    1.000000
14332                         0.138672  0.992188    5.359375
14333                         0.125854  1.005371    9.727539
14334                         0.125000  0.500000    1.000000
14335                         0.125000  0.500000    1.000000

[14336 rows x 9 columns]
```

[26]:

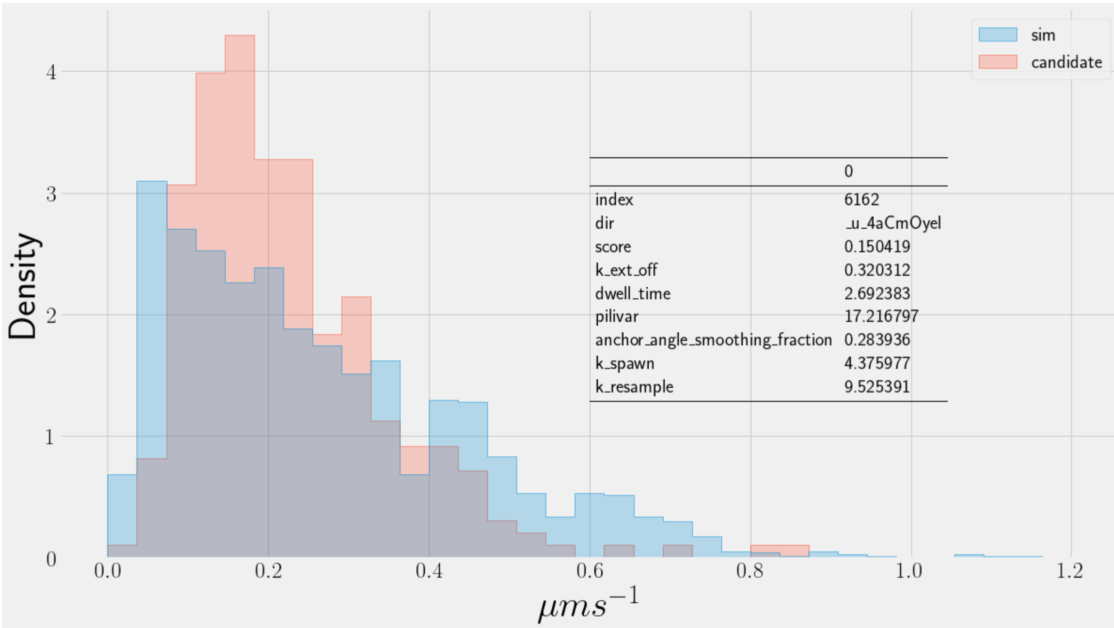
```
# sync target data from cluster here in notebook
from sobol import sync_directory
best = sortdf["top"].iloc[0]
```

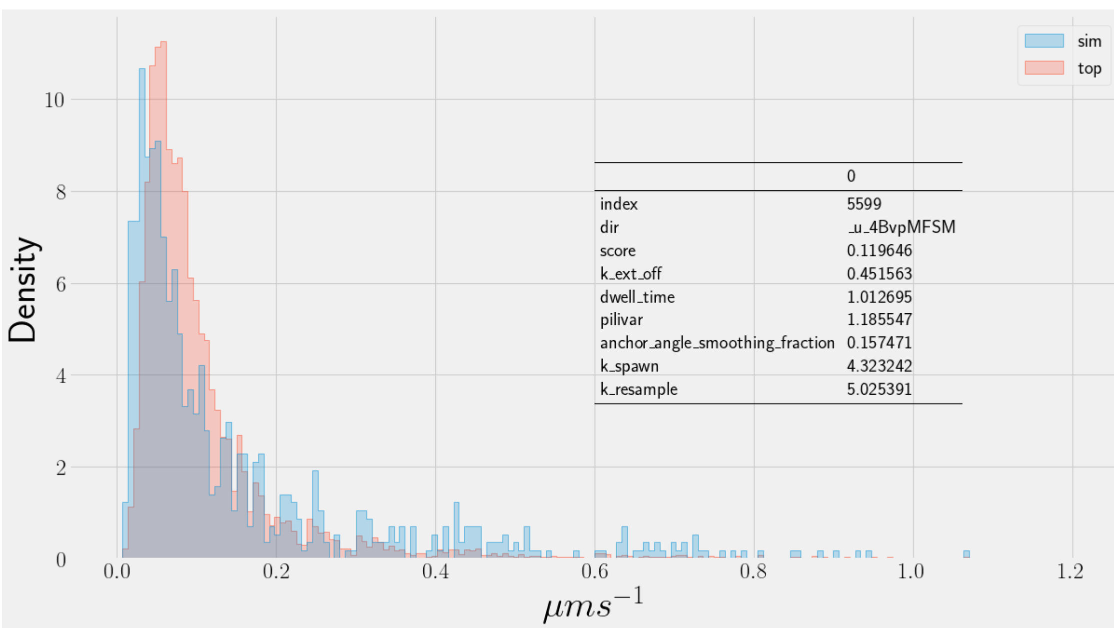
[27]:

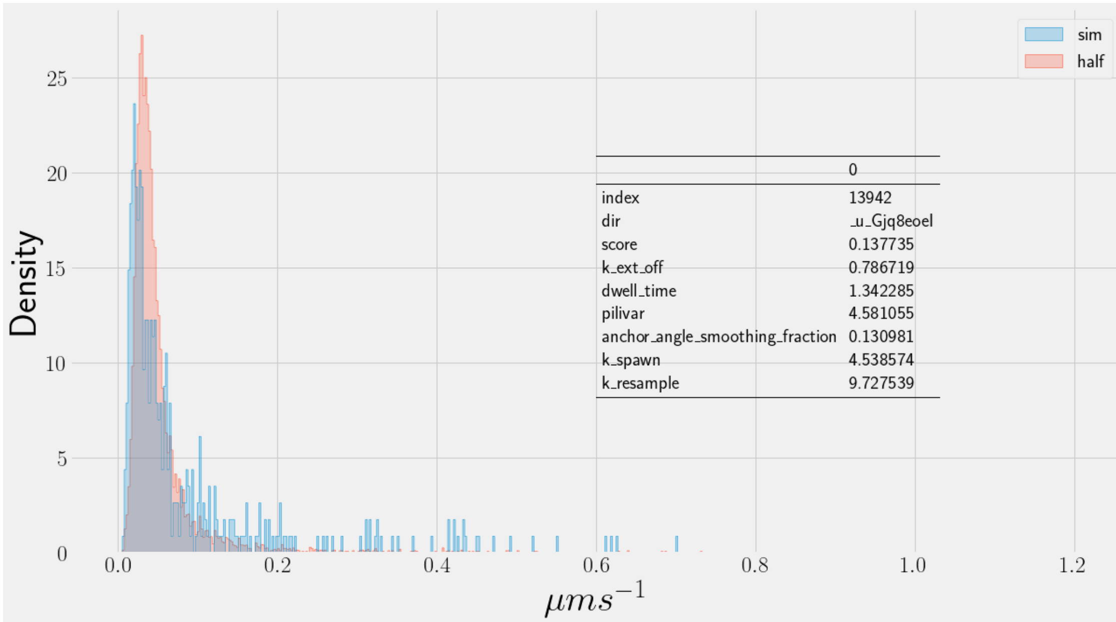
```
mpl.rcParams["text.latex.preamble"] = r'\usepackage{booktabs}'
histstyle = {"stat":"density", "common_norm": False, "element":"step"}
def plot_superimposed(dfrow, subset, simdir, histstyle=histstyle):
    target = join(simdir, dfrow["dir"])
    if not os.path.exists(join(target, "data/")):
        output = sync_directory(target)
    ltrs = twanalyse.get_linearised_data(ddir=target)
    lvel = np.concatenate([ltr.get_step_speed() for ltr in ltrs])
    xlim = (0,1.2)
    data = {"sim": lvel, subset: ref_vel[subset]}
    fig, ax = plt.subplots()
    sns.histplot(data, binrange=xlim, ax=ax, **histstyle)
    ax.text(.5,.5, dfrow.to_latex().replace('\n', ' '),
        transform=ax.transAxes, fontsize=20)
    ax.set_xlabel("$\mu ms^{-1}$")
    return ax

def plot_subset_best(sortdf, simdir):
    for subset in sortdf.keys():
        i = 0
        best = sortdf[subset].iloc[i]
```

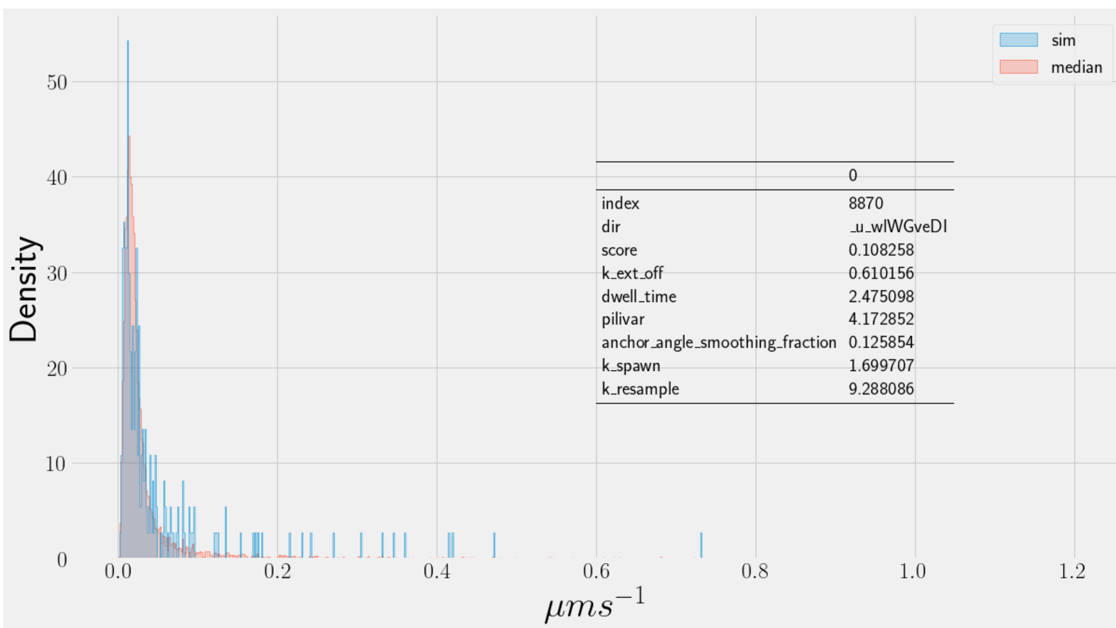
```
    plot_superimposed(best, subset, simdir, histstyle=histstyle)
```

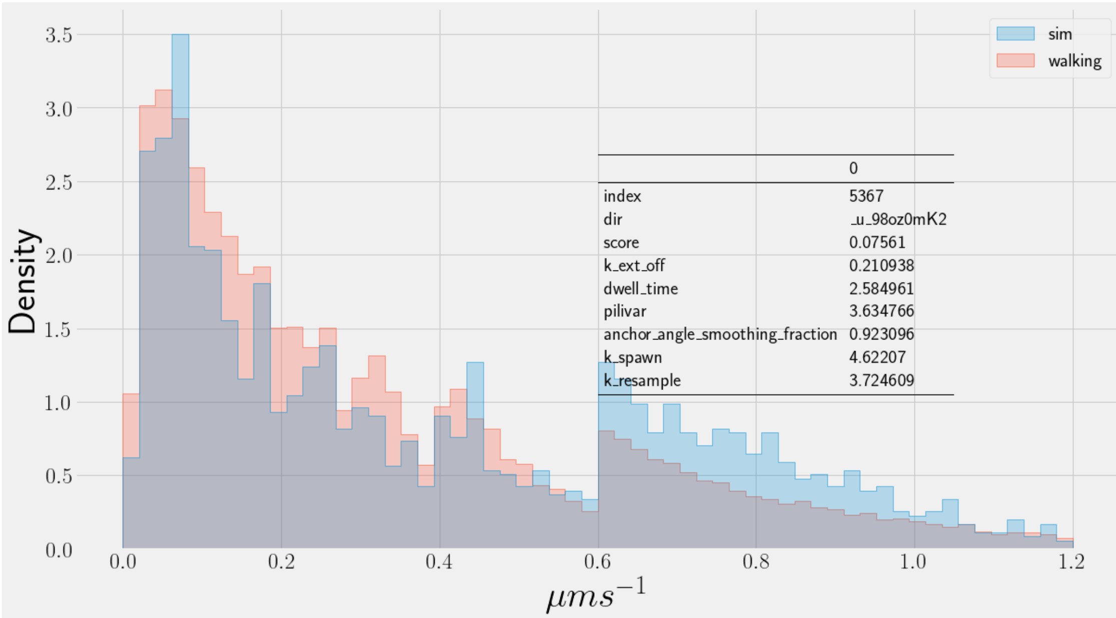
[28]:
```
plot_subset_best(sortdf, simdir)
```






sim
half
0
index 13942
dir _u_Gjq8eoel
score 0.137735
k_ext_off 0.786719
dwell_time 1.342285
pilivar 4.581055
anchor_angle_smoothing_fraction 0.130981
k_spawn 4.538574
k_resample 9.727539
Density
0 5 10 15 20 25
0.0 0.2 0.4 0.6 0.8 1.0 1.2
$\mu m s^{-1}$


sim
median
0
index 8870
dir _u_wIWGveDI
score 0.108258
k_ext_off 0.610156
dwell_time 2.475098
pilivar 4.172852
anchor_angle_smoothing_fraction 0.125854
k_spawn 1.699707
k_resample 9.288086
Density
0 10 20 30 40 50
0.0 0.2 0.4 0.6 0.8 1.0 1.2
$\mu m s^{-1}$




```
[29]: use_chi = False
      if use_chi:
          chi_scores = ['fanjin.%s.chi' % subset for subset in reference_idx.keys()]
          chi_Yf = sobol.collect_obs(lookup, lduid, subsets, chi_scores)
          chi_sortdf = sortscore(problem, lookup, chi_Yf, chi_scores)
          chi_sortdf["candidate"]
```

```
[30]: if use_chi:
          plot_subset_best(chi_sortdf, simdir)
```

```
[31]: # It's clear our chi similarity totally fails for "top" and "candidate"
      # but we know better matches exist because the ks_statistic works much better
      import scipy.stats
      check_chi = False
      if check_chi:
          _best = chi_sortdf["top"].iloc[0]
          res = 100
          ltrs = twanalyse.get_linearised_data(ddir=join(simdir, _best["dir"]))
          lvel = np.concatenate([ltr.get_step_speed() for ltr in ltrs])
          ref = ref_vel["top"]
```

```
[32]: if check_chi:
          v1 = lvel - np.mean(lvel)
          v2 = ref - np.mean(ref)
          print("mean", np.mean(lvel), np.mean(ref))
          _q = 0.050 # vary this
          xn1, xm1 =  np.quantile(v1, _q), np.quantile(v1, 1.0 - _q)
```

```python
    xn2, xm2 =  np.quantile(v2, _q), np.quantile(v2, 1.0 - _q)
    xn, xm = min(xn1, xn2), max(xm1, xm2)
    print(xn1, xm1)
    print(xn2, xm2)
    print("xlims", xn, xm)
    mspace = np.linspace(xn, xm, res)
    # method = "scott"
    def method(self):
        div_f = 4.0 # vary this
        return np.power(self.neff, -1./(self.d+4)) / div_f
    kde1 = scipy.stats.gaussian_kde(v1, bw_method=method)
    kde2 = scipy.stats.gaussian_kde(v2, bw_method=method)
    pde1 = kde1.evaluate(mspace)
    pde2 = kde2.evaluate(mspace)
    plt.plot(mspace, pde1, label="")
    plt.plot(mspace, pde2)
    chisquared = np.sum((pde2 - pde1)**2/(pde1 + pde2))
    print("chi", np.sqrt(chisquared))

    fig, ax = plt.subplots()
    sns.histplot({"sim":v1, "top":v2}, binrange=(xn, xm), **histstyle)
```

the chi metric is failing because the bandwidth is too large reducing by a factor 4 works well for this example but it may make the other examples worse (?) until we can figure out a more robust method, put trust in ks_statistic instead

[33]:
```python
simdir = "/home/dan/usb_twitching/run/5bfc8b9/cluster/sobol_walking"
lookup = sobol.read_lookup(simdir)
problem = sobol.read_problem(simdir)
print(problem)
_ , lduid = sobol.collect([], targetdir=simdir, alldata=True)
```

```
{'num_vars': 5, 'names': ['k_ext_off', 'dwell_time', 'pilivar',
'anchor_angle_smoothing_fraction', 'k_spawn'], 'bounds': [[0.2, 1.0], [0.5,
3.0], [1.0, 20.0], [0.125, 1.0], [0.1, 5.0]]}
```

[34]:
```python
import copy
_lookup = copy.deepcopy(lookup)
_lduid = copy.deepcopy(lduid)
for i, uid in reversed(list(enumerate(lookup[0]))):
    ld = lduid[uid]
    if ld.get("failed", False):
        print (uid, "failed", ld["failed_condition"])
        del _lduid[uid]
        del _lookup[1][uid]
        del _lookup[0][i]
```

```
_u_PYa0hZ5U failed step_condition
```

```
_u_ur0snpU4 failed step_condition
```

[35]:
```python
print(len(_lookup[0]), len(_lookup[1]), len(_lduid))
```

```
7166 7166 7166
```

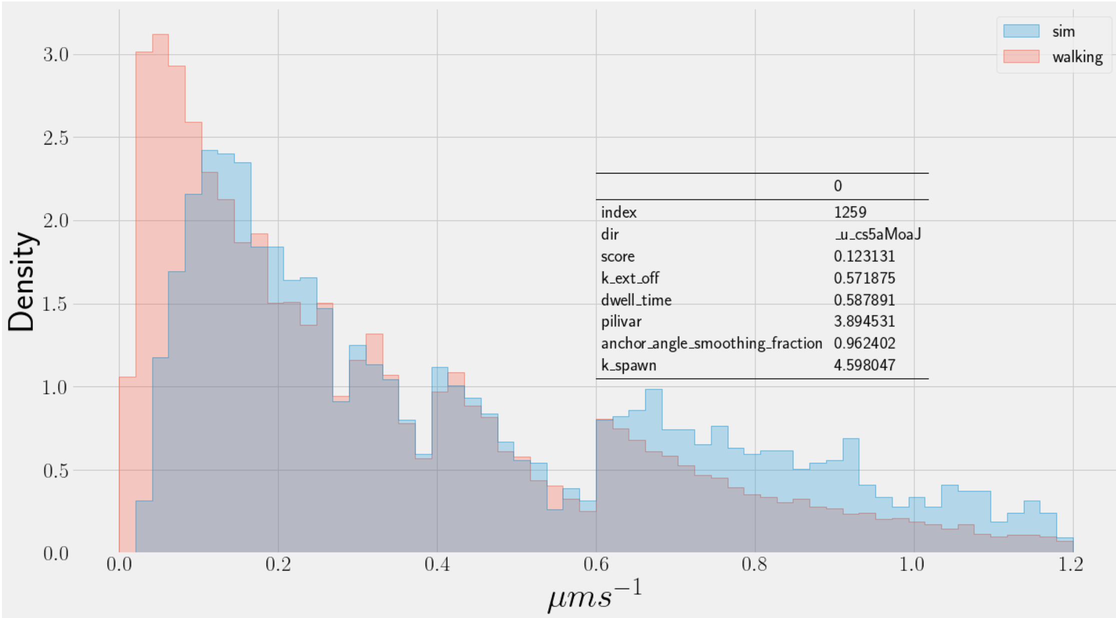
[36]:
```python
scores = ['fanjin.%s.ks_statistic' % subset for subset in reference_idx.keys()]
Yf = sobol.collect_obs(_lookup, _lduid, subsets, scores)
sortdf = sortscore(problem, _lookup, Yf, scores)
sortdf["walking"]
```

[36]:
```
      index          dir     score  k_ext_off  dwell_time    pilivar  \
0      1259  _u_cs5aMoaJ  0.123131   0.571875    0.587891   3.894531
1       886  _u_aYbIpLLa  0.130146   0.606250    0.910156   2.039062
2      3890  _u_Z1UINEcH  0.135629   0.489844    1.010254   2.206055
3      3739  _u_mN3rQZx8  0.136050   0.777344    0.736816   2.243164
4      1260  _u_WABi2BpQ  0.142264   0.678125    0.587891   3.894531
…       …          …        …         …          …          …
7161   3227  _u_Oqeg5VyP  0.684948   0.364063    2.965820  17.958984
7162   1325  _u_BJ2JoXne  0.684983   0.821875    2.619141  17.253906
7163   5186  _u_j1lsIOpn  0.685121   0.211719    2.602051  19.499023
7164   3229  _u_9VPkQBTJ  0.685987   0.864062    2.965820  15.435547
7165      6  _u_StEhhyce  0.686507   0.200000    0.500000   1.000000

      anchor_angle_smoothing_fraction   k_spawn
0                            0.962402  4.598047
1                            0.924805  4.885156
2                            0.896606  3.186426
3                            0.964966  3.109863
4                            0.962402  4.598047
…                                 …         …
7161                         0.769287  4.818164
7162                         0.142090  4.904297
7163                         0.968384  4.698535
7164                         0.769287  4.818164
7165                         0.125000  0.100000

 [7166 rows x 8 columns]
```

[37]:
```python
best = sortdf["walking"].iloc[0]
_style = copy.deepcopy(histstyle)
# _style["kde"] = True
ax = plot_superimposed(best, "walking", simdir, histstyle=_style)
plt.tight_layout()
plt.savefig("/home/dan/usb_twitching/notes/sensitivity/best_walking.png")
print("best simulation at ", join(simdir, best["dir"]))
```

```
best simulation at
```

/home/dan/usb_twitching/run/5bfc8b9/cluster/sobol_walking/_u_cs5aMoaJ



	0
index	1259
dir	_u_cs5aMoaJ
score	0.123131
k_ext_off	0.571875
dwell_time	0.587891
pilivar	3.894531
anchor_angle_smoothing_fraction	0.962402
k_spawn	4.598047

best simulation /home/dan/usb_twitching/run/5bfc8b9/cluster/sobol_walking/_u_cs5aMoaJ